

On the Coulomb interaction in superconducting pairing in cuprates

Nikolay M. Plakida

Joint Institute for Nuclear Research, 141980 Dubna, Russia

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We discuss a reduction of superconducting transition temperature by the intersite Coulomb repulsion for the d -wave pairing in cuprates. We compare the results found for the spin-fermion model and the extended Hubbard model. We argue that in both the models the d -wave superconducting transition temperature is reduced by the Coulomb repulsion of holes in different unit cells. We also show that in the strong correlation limit the s -wave superconductivity cannot occur due to the kinematic restriction of no double occupancy in the Hubbard subbands.

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It is commonly believed that the Coulomb interaction is detrimental to superconductivity. In particular, for low-temperature superconductors with the s -wave pairing mediated by electron-phonon coupling the retardation effect renormalizes the Coulomb interaction which makes it feasible to obtain a finite superconducting T_c [1, 2]. For electronic pairing mechanisms, the retardation effect is ineffective and the Coulomb interaction suppresses the s -wave pairing. Only superconducting pairing with higher orbital momenta, p, d, f, \dots , can occur in the Fermi-liquid as originally was proposed by Kohn and Luttinger [3] (for a review see [4]).

The cuprate superconductors are the Mott-Hubbard (more accurately, charge-transfer) doped insulators caused by the large Coulomb interaction U_d on copper sites. In this case the interaction U_d should be taken into account rigorously in considering the electronic structure of cuprates. The most frequently used is the three-band p - d model for Cu $3d(x^2-y^2)$ -states and O $2p_\sigma(x, y)$ -states in the CuO₂ plane [5, 6]. To obtain a tractable model for description of low-energy electronic excitations the p - d model can be reduced to simpler models.

In particular, in the spin-fermion model (SFM) the high-energy excitations on copper sites are excluded, which results in a conduction band for oxygen holes on the O $2p_\sigma(x, y)$ orbitals interacting with localized copper spins $S = 1/2$ in the CuO₂ plane (see, e.g., [7]). In Ref. [8], the SFM was used to consider the d -wave superconducting pairing for spin-polarons. It was found that the Coulomb interaction V_{pp} between holes on the nearest neighbor oxygen sites gives no contribution to the d -wave pairing by symmetry reason. This was considered as a proof of stability of the d -wave pairing towards the intersite Coulomb repulsion. However, the authors have neglected the Coulomb interaction between holes in different unit cells, which conventionally reduces the superconducting T_c .

Another approach is based on the cell-cluster perturbation theory (see [9–13]). In the theory, the spectrum of electronic excitations in the unit cell CuO₄ is rigorously calculated by an exact diagonalization of the copper and oxygen energy states taking into account all relevant Coulomb interactions, U_d, U_p, V_{pd}, V_{pp} , and hybridiza-

tions, t_{pd}, t_{pp} . Considering the lowest energy states close to the Fermi level, the singly occupied $d(x^2 - y^2)$ states and doubly occupied singlet p - d hole states, the extended Hubbard model (EHM) can be formulated for two Hubbard subbands with the hopping parameter between different unit cells $t \sim 0.3t_{pd}$ and the intersite Coulomb repulsion $V \sim 0.5t$ [11].

In the limit of strong correlations the projected (Hubbard) electronic operators should be used [14]. They have nonfermionic commutation relations, as e.g., the commutation relation for the Hubbard operators in the singly occupied subband, $X_i^{0\sigma} = a_{i\sigma}(1 - N_{i\bar{\sigma}})$ where $N_{i\sigma} = a_{i\sigma}^\dagger a_{i\sigma}$, $\sigma = \pm 1$, $\bar{\sigma} = -\sigma$, reads

$$X_i^{0\sigma} X_j^{\sigma 0} + X_j^{\sigma 0} X_i^{0\sigma} = \delta_{ij}(1 - N_{i\sigma}/2 + \sigma S_i^z). \quad (1)$$

This results in the kinematic interaction for electrons, which is determined by electron scattering on charge (number $N_{i\sigma}$) and spin S_i^α fluctuations with the coupling of an order of the hopping parameter t .

In Refs. [15, 16], the EHM was studied within the strong coupling superconducting theory. It was shown that the spin-fluctuation pairing induced by the kinematical interaction in the second order of t results in the d -wave superconductivity with high- T_c . In Ref. [15], it was found that the intersite Coulomb repulsion $V \sim 0.5t$ in cuprates is not strong enough to suppress the d -wave superconductivity. To prove this pairing mechanism, in Ref. [16] we consider a much stronger than in cuprates Coulomb interaction V . Only for V larger than the coupling constant for the spin-fluctuation pairing, $V \gtrsim 4t$, the d -wave pairing can be fully suppressed.

Now we comment on the s -wave superconducting pairing in cuprates. The s -wave pairing induced by the kinematical interaction in the limit of strong correlations was originally proposed in Refs. [17]. In Refs. [18, 19], the superconducting pairing in the two-dimensional Hubbard model was studied. It was found that this pairing is robust in respect to the intersite Coulomb interaction V . However, in these papers only the first order of the kinematical interaction $\propto t$ was considered, which results in the s -wave pairing with the symmetric superconducting gap $\Delta_\sigma(q_x, q_y) = \Delta_\sigma(q_y, q_x)$. However, in this

case the well known constraint of “no double occupancy” in strongly correlated systems is violated. First, it was pointed out in Refs. [20, 21] for the t - J model and then in Ref. [16] for the EHM model. This constraint can be formulated in terms of a specific relation for the anomalous (pair) correlation function for the Hubbard operators. It is easy to verify that a product of two Hubbard operators for the singly occupied subband equals zero: $X_i^{0\sigma} X_i^{0\bar{\sigma}} = a_{i\sigma}(1 - N_{i\bar{\sigma}}) a_{i\bar{\sigma}}(1 - N_{i\sigma}) = 0$. Therefore, the corresponding single-site pair correlation function should vanish:

$$F_{ii,\sigma} = \langle X_i^{0\sigma} X_i^{0\bar{\sigma}} \rangle = \frac{1}{N} \sum_{\mathbf{q}} \langle X_{\mathbf{q}}^{0\sigma} X_{-\mathbf{q}}^{0\bar{\sigma}} \rangle \equiv 0. \quad (2)$$

The symmetry of the Fourier-component of the pair correlation function $F_{\sigma}(\mathbf{q}) = \langle X_{\mathbf{q}}^{0\sigma} X_{-\mathbf{q}}^{0\bar{\sigma}} \rangle$ has the symmetry of the superconducting order parameter, i.e., the gap function. For the tetragonal lattice for the d -wave pairing $F_{\sigma}(q_x, q_y) = -F_{\sigma}(q_y, q_x)$ and the condition (2) after integration over q_x, q_y is fulfilled. For the s -wave pairing $F_{\sigma}(q_x, q_y) = F_{\sigma}(q_y, q_x)$ and the condition (2) is violated. The same condition holds for the pair correlation function for the second Hubbard subband, $\langle X_i^{\sigma 2} X_i^{\bar{\sigma} 2} \rangle = 0$. Therefore, the s -wave pairing in both the Hubbard subbands is prohibited in the limit of strong correlations.

To overcome the restriction (2) in Refs. [22] it was proposed to consider the modified time-dependent pair correlation function:

$$\tilde{F}_{ii,\sigma}(t) = \int_{-\infty}^{+\infty} d\omega e^{i\omega t} \tilde{J}_{ii,\sigma}(\omega), \quad (3)$$

where

$$\tilde{J}_{ii,\sigma}(\omega) = J_{ii,\sigma}(\omega) - \delta(\omega) \int_{-\infty}^{+\infty} d\omega_1 J_{ii,\sigma}(\omega_1). \quad (4)$$

The spectral density $J_{ii,\sigma}(\omega)$ determines the original correlation function

$$F_{ii,\sigma}(t) = \langle X_i^{0\sigma}(t) X_i^{0\bar{\sigma}} \rangle = \int_{-\infty}^{+\infty} d\omega e^{i\omega t} J_{ii,\sigma}(\omega). \quad (5)$$

For the modified spectral density (4) the condition (2) is trivially satisfied for any spectral function $J_{ii,\sigma}(\omega)$ and the restriction on the s -wave pairing seems to be lifted.

However, thy spectral density (4) results in the nonergodic behavior [23] of the pair correlation function (3):

$$C_{ii,\sigma} = \lim_{t \rightarrow \infty} \tilde{F}_{ii,\sigma}(t) = -\frac{1}{N} \sum_{\mathbf{q}} \langle X_{\mathbf{q}}^{0\sigma} X_{-\mathbf{q}}^{0\bar{\sigma}} \rangle, \quad (6)$$

where the conventional pair correlation function decays in the limit $t \rightarrow \infty$ due to finite life-time effects

$$\lim_{t \rightarrow \infty} F_{ii,\sigma}(t) = \int_{-\infty}^{+\infty} d\omega e^{i\omega t} J_{ii,\sigma}(\omega) = 0. \quad (7)$$

The nonergodic behavior of the modified pair correlation function (3) contradicts the basic properties of physical systems and appears for some pathological models with local integrals of motion [24, 25]. In that case, the nonergodic constants can be found from $1/\omega$ poles of the anticommutator or causal Green functions, as described for the Hubbard model for spin or charge excitations in Refs. [26, 27] contrary to the arbitrary definition (4). Therefore, the statement given in Refs. [22]: “The inclusion of a singular contribution to the spectral intensity of the anomalous correlation function regains the sum rule and remove the unjustified forbidding of the s -symmetry order parameter in superconductors with strong correlations” cannot be accepted.

To conclude, the contradiction between the theoretical and experimental results claimed in Ref. [8]: a more stable s -wave superconducting pairing with respect to the intersite Coulomb interaction found in Refs. [18, 19], and a strong suppression of the d -wave pairing found in Refs. [15, 16], in fact, is absent. The s -wave pairing in the limit of strong correlations is prohibited due to the kinematical restriction (2), while the d -wave pairing found within the EHM can be suppressed only for unphysically large Coulomb interaction V , as shown in Refs. [16]. The cancellation of the intersite Coulomb interaction for the d -wave pairing in SFM was found in Ref. [8] only for the nearest-neighbor oxygen sites, which does not prevent suppression of d -wave pairing due to the Coulomb interaction for oxygen sites in different unit cells as in EHM.

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